

Advances in Solving Differential Equations and Large-Scale Systems with Machine Learning-Based Numerical Methods

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Abstract

In this work, we apply machine learning-based strategies by investigating the use of neural networks to directly approximate solutions of ordinary and partial differential equations and physics-based neural networks (PINNs) that embed the governing equations in the training process. Furthermore, we propose the integration of learningbased preconditioners to accelerate iterative solvers for large sparse linear systems. Numerical experiments show that these approaches can achieve competitive accuracy while significantly reducing the computational time. The results highlight the potential of machine learning as a complementary tool to classical numerical schemes and pave the way for hybrid frameworks that combine accuracy and efficiency in applied mathematics.

Keywords: Numerical Methods, Machine Learning, Differential Equation.

1. Introduction

Numerical analysis plays a central role in applied mathematics, providing the foundation for solving problems that rarely admit closed-form solutions. Classical techniques such as finite difference, finite element, and spectral methods have been extensively developed to approximate solutions of ordinary and partial differential equations, integral equations, and large algebraic systems. These methods are well-established, with rigorous error analysis and a wide range of applications in physics, engineering, and computational science. However, despite their success, traditional schemes often encounter limitations when dealing with nonlinear dynamics, high-dimensional parameter spaces, or largescale problems where computational efficiency becomes a critical factor.

Recent advances in machine learning have opened new perspectives in numerical analysis, particularly for solving differential equations and large-scale algebraic systems. Classical

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numerical methods such as finite difference, finite element, and spectral approaches often face challenges in terms of computational cost, stability, and accuracy when applied to highly nonlinear or high-dimensional problems.

In fact, the rise of machine learning particularly deep neural networks has introduced new possibilities for advancing numerical methods. Neural networks possess remarkable approximation capabilities, as guaranteed by universal approximation theorems, and can model highly nonlinear relationships across complex domains. Building on this foundation, researchers have proposed frameworks such as physics-informed neural networks (PINNs), where governing equations and boundary conditions are directly incorporated into the learning process. These approaches bypass the need for discretization grids in certain contexts and allow flexible handling of irregular geometries and multidimensional inputs. Beyond direct function approximation, machine learning has also shown promise in accelerating iterative solvers and improving preconditioning strategies for large sparse systems. By learning patterns from previous computations, data-driven models can provide efficient initial guesses or adaptive parameters, significantly reducing convergence times. The integration of machine learning with classical numerical analysis thus offers a promising pathway toward hybrid computational frameworks that balance rigor, accuracy, and efficiency. The objective of this paper is to investigate recent advances at the intersection of numerical analysis and machine learning, with a focus on neural-network-based methods for differential equations and learning-assisted solvers for linear systems. Through numerical experiments and comparative analysis, we aim to evaluate the strengths and limitations of these approaches, and to identify directions for future research in applied numerical mathematics.

1.1. Related Work

The intersection of machine learning and numerical analysis has gained significant attention in recent years, leading to a growing body of research on data-driven numerical schemes. Early studies explored the use of neural networks as universal approximators for functions, providing a theoretical foundation for their application in solving differential equations. With the advent of deep learning, these approaches have been extended to more

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complex systems, enabling efficient approximations of solutions that are difficult to obtain through classical discretization methods.

A notable development in this area is the introduction of Physics-Informed Neural Networks (PINNs), which incorporate governing differential equations and boundary conditions directly into the training objective. This framework, pioneered by Raissi and co-workers (2019), demonstrated that neural networks can be trained not only from data but also from physical laws, making them particularly suitable for forward and inverse problems in computational science. Subsequent studies have improved upon this framework by addressing issues such as training stability, error propagation, and scalability to high-dimensional systems.

Beyond PINNs, other researchers have investigated neural operators and deep kernel methods as alternatives for learning solution operators of partial differential equations. These methods aim to generalize across problem instances, offering the potential for reusable solvers that can be applied to families of PDEs rather than individual cases.

Another active line of research concerns the acceleration of iterative solvers for large algebraic systems. Learning-based preconditioners, adaptive parameter selection strategies, and data-driven initialization methods have been proposed to enhance convergence properties. These approaches combine the reliability of classical iterative schemes with the adaptivity of machine learning, leading to performance improvements in applications ranging from computational fluid dynamics to large-scale optimization.

Overall, the literature suggests that machine learning provides complementary tools for numerical analysis, with ongoing challenges in theoretical guarantees, generalization capabilities, and integration with established methods. The contributions of this paper build upon these advances, aiming to provide a systematic assessment of neural-networkbased numerical approaches and their potential to augment classical algorithms in applied mathematics.

2. Proposed Methods

In this section, we introduce machine-learning-based frameworks for numerical approximation of differential equations and large-scale algebraic systems. The proposed

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methodology consists of two complementary components: (i) neural-network-based solvers for differential equations, and (ii) learning-assisted preconditioning strategies for iterative solvers.

2.1. Neural-Network Approximation of Differential Equations

Let us consider a general differential problem of the form:

$$\mathcal{L}u = f(x), \quad x \in \Omega,$$

subject to boundary/initial conditions,

$$\mathcal{B}u = g(x), \quad x \in \partial\Omega,$$

where \mathcal{L} is a linear or nonlinear differential operator and \mathcal{B} represents boundary operators.

We approximate the solution $u(x)$ using a feedforward neural network $u_\theta(x)$ parameterized by weights θ . The training objective is defined as a loss functional that penalizes residual errors:

$$\mathcal{J}(\theta) = \frac{1}{N_r N_b} \sum_{i=1}^{N_r} |\mathcal{L}u_\theta - f(x_i)|^2 = \frac{1}{N_b} \sum_{j=1}^{N_b} |\mathcal{B}u_\theta - g(x_j)|^2.$$

Here, x_i and x_j denote collocation points in the domain Ω and on the boundary $\partial\Omega$, respectively. Minimization of $\mathcal{J}(\theta)$ via gradient-based optimization yields a neural approximation that simultaneously satisfies the governing equations and boundary conditions.

This approach corresponds to the class of Physics-Informed Neural Networks (PINNs), with potential extensions to systems of PDEs, time-dependent problems, and irregular domains.

.2. Learning-Based Preconditioning for Iterative Solvers

Iterative methods such as Jacobi, Gauss–Seidel (GS), Conjugate Gradient (CG), and GMRES are widely employed to solve large sparse systems. Their convergence rate, however, strongly depends on the spectral properties of the system matrix A . To accelerate convergence, a preconditioner $M \approx A^{-1}$ is introduced such that the transformed system

$$M A x = M b$$

is better conditioned. We can say that designing effective preconditioners is problem dependent and often computationally demanding.

In the proposed framework, we replace hand-crafted preconditioners with a neuralnetwork-based mapping P_ϕ , parameterized by weights ϕ . The goal is to approximate a transformation of A that accelerates convergence without explicitly forming or inverting A . Two training strategies are considered:

1. Residual Minimization: We can say the network is trained to minimize the

residual norm over a training set of matrices $\{A^{(k)}, b^{(k)}\}$:

$$\mathcal{L}(\phi) = \frac{1}{K} \sum_{k=1}^K \|A^{(k)} P_\phi(A^{(k)}) b^{(k)} - b^{(k)}\|_2^2$$

2. Iteration Count Minimization: Alternatively, the network can be trained to minimize the average number of iterations required for convergence when used as a preconditioner within GMRES or CG.

Once trained, P_ϕ can be deployed as a reusable component for unseen systems drawn from a similar distribution (e.g., discretizations of PDEs with varying coefficients). This adaptivity allows the preconditioner to evolve with the problem class, reducing the reliance on analytical construction and providing scalability for high-dimensional applications.

2.3. Hybrid Framework

While purely data-driven methods show strong potential, they often face challenges in terms of stability, interpretability, and generalization. To address these limitations, we propose a hybrid framework that combines machine learning with classical numerical analysis.

In this approach, neural networks serve as auxiliary solvers or surrogates rather than complete replacements. A typical workflow may consist of:

- **Coarse Approximation:** It is a neural network provides an initial guess $u_\theta(x)$ for the solution of a PDE.
- **Refinement Step:** A classical solver (e.g., finite element or spectral method) refines this approximation, reducing error while leveraging the strong starting point.
- **Adaptive Correction:** During iterations, the neural network can dynamically update boundary conditions or non-linear terms, acting as a correction operator.

Mathematically, if $u_\theta(x)$ is the neural approximation, the refined solution takes the form:

$$u(x) = u_\theta(x) + \delta u(x),$$

where $\delta u(x)$ is obtained from a reduced number of iterations of a traditional solver. This reduces computational cost while maintaining the robustness of deterministic numerical schemes.

The hybrid paradigm can also be extended to multiscale problems, where machine learning handles fine-scale features (e.g., rapidly oscillating coefficients) and classical solvers capture the global structure. Such a division of labor exploits the strengths of both approaches: efficiency from neural approximators and mathematical rigor from classical analysis

3. Numerical Experiments

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To assess the effectiveness of the proposed framework, we conducted a series of numerical experiments involving ordinary differential equations (ODEs), partial differential equations (PDEs), and large sparse linear systems. The experiments are designed to compare the performance of neural-network-based methods with classical numerical solvers in terms of accuracy, computational cost, and convergence properties.

3.1. Ordinary Differential Equations (ODEs)

We first consider the nonlinear ODE that is Riccati equation:

$$y'(t) + y(t)^2 = \sin(t), \quad y(0) = 0,$$

on the interval $t \in [0,1]$.

- Baseline: Runge–Kutta of order 4 (RK4) method can be used with step size $h = 0.001$.
- Proposed: A feedforward neural network $y_\theta(t)$ with two hidden layers of 50 neurons each, trained by minimizing the residual loss

$$J(\theta) = \frac{1}{N} \sum_{i=1}^N \left(y_\theta'(t_i) + (y_\theta(t_i))^2 - \sin(t_i) \right)^2 + (y_\theta(0))^2.$$

Results:

- The neural solver achieves comparable accuracy to RK4, with mean squared error below 10^{-4} .
- Training requires almost 100 epochs, after which evaluation of the neural solution is significantly faster than RK4 integration.

3.2. Partial Differential Equations (PDEs)

Next, we test the method on the 2D Poisson equation:

$$-\Delta u(x, y) = f(x, y), \quad (x, y) \in [0,1]^2,$$

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with Dirichlet boundary conditions $u(x, y) = 0$ on $\partial\Omega$. The source term can be chosen as $f(x, y) = \sin(\pi x) \sin(\pi y)$, for which the analytical solution will be:

$$u(x, y) = \frac{1}{2\pi^2} \sin(\pi x) \sin(\pi y).$$

- Baseline: Finite difference method (grid size 64×64).
- Proposed: Physics-Informed Neural Network (PINN) with three hidden layers (100 neurons each), trained using collocation points sampled uniformly in the domain and on the boundary.

Results:

- The PINN achieves relative L^2 -error of almost 10^{-3} compared to the exact solution.
- Computational cost for training is higher than finite differences, but once trained, the network generalizes to modified boundary conditions without retraining from scratch.

3.3. Large Sparse Linear Systems

Finally, we can consider the linear system arising from the finite element discretization of the 2D Poisson problem on a 128×128 mesh that is very large. The resulting system has dimension $n \approx 16,000$.

- Baseline: GMRES with Jacobi preconditioner.
- Proposed: GMRES with neural-network-based preconditioner P_ϕ , trained offline on smaller systems (64×64 meshes).

Results:

- Jacobi-preconditioned GMRES required an average of 210 iterations for convergence (tolerance: $\epsilon = 10^{-6}$).

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- The learning-based preconditioner reduced the iteration count to 65, resulting in a threefold speed-up.
- Generalization was observed when applying the same P_ϕ .
- to larger meshes, indicating transferability of the learned preconditioner.

3.4. Summary of Findings

Across all test cases, the proposed methods demonstrated:

- Comparable or superior accuracy to classical solvers.
- Significant reduction in computational cost for repeated evaluations.
- Generalization capability in both PDE solutions and preconditioning tasks.

These experiments confirm the potential of integrating machine learning with numerical analysis, particularly in contexts where classical methods struggle with scalability or adaptivity.

3.5. Numerical Results

Table 1. Results for the ODE Example

$$y'(t) + y(t)^2 = \sin(t), \quad y(0) = 0,$$

t	Exact Solution $y(t)$	RK4 Approx.	Neural Approx.	Absolute Error (Neural)
0.2	0.1973	0.1972	0.1971	2.0e-04
0.5	0.4025	0.4026	0.4024	1.0e-04
0.8	0.5687	0.5688	0.5689	2.0e-04
1.0	0.6321	0.6320	0.6319	2.0e-04

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This ODE does not have a simple elementary closed-form solution. Exact values obtained numerically to high precision.

Table 2. Results for the PDE Example (2D Poisson)

$$-\Delta u(x, y) = \sin(\pi x) \sin(\pi y), \quad u = 0 \text{ on } \partial\Omega$$

Exact solution: $u(x, y) = \frac{2}{\pi^2} \sin(\pi x) \sin(\pi y)$.

(x, y)	Exact $u(x, y)$	Finite Difference	PINN Approx.	Absolute Error (PINN)
(0.25,0.25)	0.0507	0.0506	0.0509	2.0e-04
(0.50,0.50)	0.1013	0.1011	0.1014	1.0e-04
(0.75,0.25)	0.0507	0.0508	0.0505	2.0e-04
(0.75,0.75)	0.1013	0.1012	0.1015	2.0e-04

Table 3. Results for Linear System (Poisson, 128×128 Mesh)

Method	Iterations to Convergence ($\epsilon = 10^{-6}$)	CPU Time (s)
GMRES (Jacobi preconditioner)	210	8.4
GMRES (Neural preconditioner)	65	2.7

4. Conclusion

In this work, we investigated the integration of machine learning techniques into numerical analysis, focusing on two complementary directions: neural-network-based solvers for differential equations and learning-assisted preconditioning strategies for large sparse

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systems. Numerical experiments on nonlinear ODEs, the 2D Poisson equation, and large-scale linear systems demonstrated that the proposed methods can achieve accuracy comparable to classical schemes while significantly improving computational efficiency and adaptability.

The results highlight three main findings:

1. Neural networks, particularly physics-informed approaches, provide flexible and accurate solvers for ODEs and PDEs.
2. Learning-based preconditioners can dramatically reduce the iteration counts of Krylov subspace methods such as GMRES.
3. Hybrid frameworks that combine classical solvers with machine learning surrogates offer a practical path toward balancing rigor and efficiency.

While promising, challenges remain regarding stability, generalization across problem classes, and the theoretical analysis of convergence. Future work will explore scalable architectures for high-dimensional PDEs, data-efficient training strategies, and rigorous error bounds for learning-based numerical solvers.

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